Virtual design and development of novel electrode concepts for Lithium-Ion batteries

Li-Ion batteries are commonly used in portable electronic devices due to their outstanding energy and power density. However, in order to reach the requirements of the automotive industry for next-generation electric vehicles regarding safety, life-time, energy density, and rate capability further developments are inevitable. Additionally, a reduction of material and production costs is needed to further increase the market penetration of electric vehicles. Currently, several novel cell chemistries[1] based on abundant materials such as magnesium[2] and sodium[3] are under investigation, however, at the moment Li-Ion batteries are the only commercial product coming close to the requirements specified above.
The capacity of state-of-the-art Li-Ion batteries is intrinsically limited by its intercalation chemistry [4]. During charge and discharge of the battery lithium ions are shuttling between the positive and negative electrode where they are inserted in the host structure of the active materials. In order to improve the energy density the share of inactive materials such as separators, current collectors, housing, etc. needs to be reduced. This can be done by either making these components thinner, which bears some safety risks, or by increasing the areal capacity and/or thickness of the electrode layers. The latter approach has the advantage that less electrode layers are needed to assemble a battery of the same capacity which also reduces production time and cost. However, increasing the active material loading can cause transport limitations[5] of the shuttling lithium ions which limits the rate capability of the cell and, thus, is problematic for the targets of the automotive industry regarding fast charging. Moreover, new cell designs and production methods[6,7] might need to be developed.
A possible route towards high capacity electrodes for Li-Ion batteries is the development of new structuring techniques by e.g. laser perforation. Computer simulations can be a very useful and versatile tool to find optimal cell designs or electrode structures. Our virtual design approach is based on 3D micro-structure resolved simulations in the in-house software package BEST (Battery and Electrochemistry Simulation Tool)[8]. The governing conservation equations for mass, charge, and energy were derived in an approach based on non-equilibrium thermodynamics[9] and allow tracking important quantities like the local concentration of lithium in the electrolyte and active material or the temperature distribution in the cell. Based on this information limiting processes for the global battery performance or life-time can be detected and different electrode designs can be evaluated. An important basis for predictive simulations is a sound parameterization of the model. Electrochemical parameters and transport parameters can be determined in independent model experiments and a brief overview of the methodology will be given[10].
The second corner stone of the simulations are the electrode structures themselves. Virtual electrode structures are obtained by tomographic methods like Focused Ion Beam - Scanning Electron Microscopy (FIB-SEM) and x-ray Computed Tomography (CT) or virtual stochastic 3D geometry generators[11]. The latter are parametrized with tomography data and allow exploring a large parameter space of realistic electrode structures. This methodology gives the opportunity to correlate material and structural properties with the performance of the battery and therefore, provides an important design tool for the processing of improved electrode geometries.
In the presentation a short introduction to the fundamentals and working principles of Li-Ion batteries will be given. A focus will be set on current limitations and future targets. In the second part I will introduce the virtual design approach developed in our group and demonstrate the capabilities of the approach with the help of a few selected design studies of novel electrode processing concepts.

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